

*Project-Team IPSO**Invariant Preserving Solvers**Rennes*

THEME NUM

Activity
Report

2004

Table of contents

1. Team	1
2. Overall Objectives	1
2.1. An overview of geometric numerical integration	1
2.2. Overall objectives	1
3. Scientific Foundations	2
3.1. Structure-preserving numerical schemes for solving ordinary differential equations	2
3.1.1. Reversible ODEs	2
3.1.2. ODEs with an invariant manifold	3
3.1.3. Hamiltonian systems	3
3.1.4. Differential-algebraic equations	4
3.2. Highly-oscillatory systems	4
3.3. Geometric schemes for the Schrödinger equation	5
3.4. High-frequency limit of the Helmholtz equation	6
3.5. From the Schrödinger equation to Boltzmann-like equations	6
3.6. Spatial approximation for solving ODEs	7
4. Application Domains	7
4.1. Laser physics	7
4.2. Molecular Dynamics	8
5. New Results	8
5.1. Long-time averages for molecular simulations	8
5.2. Constrained Hamiltonian systems and differential-algebraic systems	9
5.3. A Poisson system with boundary conditions	9
5.4. Gaussian wave packets	10
5.5. Energy conservation	11
5.6. From the Bloch model to the rate equations	11
5.7. From the Schrödinger to the Boltzmann equation	12
5.8. High frequency limit of the Helmholtz equation	12
5.9. An algebraic approach to invariant preserving integrators	12
5.10. Shell theory	13
5.11. Spatial approximation for solving ODEs	13
6. Contracts and Grants with Industry	14
7. Other Grants and Activities	15
7.1. National Grants	15
7.1.1. ARC PRESTISSIMO 2003-2004	15
7.1.2. ACI Molecular Simulation 2004-2007	15
7.1.3. ACI High-frequency methods for ordinary and partial differential equations 2003-2006	16
8. Dissemination	16
8.1. Program committees, editorial Boards and organization of conferences	16
8.2. INRIA and University committees	16
8.3. Teaching	17
8.4. Participation in conferences	17
8.5. International exchanges	17
8.5.1. Visits	17
8.5.2. Visitors	17
9. Bibliography	18

1. Team

Head of project-team

Philippe Chartier [DR Inria]

Administrative assistant

Fabienne Cuyollaa [TR Inria]

Staff members

Erwan Faou [CR Inria]

Faculty members

François Castella [PROF., University of Rennes 1, délégation INRIA]

Research scientists

Michel Crouzeix [PROF., University of Rennes 1]

2. Overall Objectives

2.1. An overview of geometric numerical integration

A fundamental and enduring challenge in science and technology is the quantitative prediction of time-dependent nonlinear phenomena. While dynamical simulation (for ballistic trajectories) was one of the first applications of the digital computer, the problems treated, the methods used, and their implementation have all changed a great deal over the years. Astronomers use simulation to study long term evolution of the solar system. Molecular simulations are essential for the design of new materials and for drug discovery. Simulation can replace or guide experiment, which often is difficult or even impossible to carry out as our ability to fabricate the necessary devices is limited.

During the last decades, we have seen dramatic increases in computing power, bringing to the fore an ever widening spectrum of applications for dynamical simulation. At the boundaries of different modeling regimes, it is found that computations based on the fundamental laws of physics are under-resolved in the textbook sense of numerical methods. Because of the vast range of scales involved in modeling even relatively simple biological or material functions, this limitation will not be overcome by simply requiring more computing power within any realistic time. One therefore has to develop numerical methods which capture crucial structures even if the method is far from “converging” in the mathematical sense. In this context, we are forced increasingly to think of the numerical algorithm as a part of the modeling process itself. A major step forward in this area has been the development of structure-preserving or “geometric” integrators which maintain conservation laws, dissipation rates, or other key features of the continuous dynamical model. Conservation of energy and momentum are fundamental for many physical models; more complicated invariants are maintained in applications such as molecular dynamics and play a key role in determining the long term stability of methods. In mechanical models (biodynamics, vehicle simulation, astrodynamics) the available structure may include constraint dynamics, actuator or thruster geometry, dissipation rates and properties determined by nonlinear forms of damping.

In recent years the growth of geometric integration has been very noticeable. Features such as *symplecticity* or *time-reversibility* are now widely recognized as essential properties to preserve, owing to their physical significance. This has motivated a lot of research [33][27][26] and led to many significant theoretical achievements (symplectic and symmetric methods, volume-preserving integrators, Lie-group methods, ...). In practice, a few simple schemes such as the Verlet method or the Störmer method have been used for years with great success in molecular dynamics or astronomy. However, they now need to be further improved in order to fit the tremendous increase of complexity and size of the models.

2.2. Overall objectives

To become more specific, the project *IPSO* aims at finding and implementing new structure-preserving schemes and at understanding the behavior of existing ones for the following type of problems:

- systems of differential equations posed on a manifold.
- systems of differential-algebraic equations of index 2 or 3, where the constraints are part of the equations.
- Hamiltonian systems and constrained Hamiltonian systems (which are special cases of the first two items though with some additional structure).
- highly-oscillatory systems (with a special focus of those resulting from the Schrödinger equation).

Although the field of application of the ideas contained in geometric integration is extremely wide (e.g. robotics, astronomy, simulation of vehicle dynamics, biomechanical modeling, biomolecular dynamics, geodynamics, chemistry...), *IPSO* will mainly concentrate on applications for *molecular dynamics simulation* and *laser simulation*:

- There is a large demand in biomolecular modeling for models that integrate microscopic molecular dynamics simulation into statistical macroscopic quantities. These simulations involve huge systems of ordinary differential equations over very long time intervals. This is a typical situation where the determination of accurate trajectories is out of reach and where one has to rely on the good qualitative behavior of structure-preserving integrators. Due to the complexity of the problem, more efficient numerical schemes need to be developed.
- The demand for new models and/or new structure-preserving schemes is also quite large in laser simulations. The propagation of lasers induces, in most practical cases, several well-separated scales: the intrinsically highly-oscillatory *waves* travel over long distances. In this situation, filtering the oscillations in order to capture the long-term trend is what is required by physicists and engineers.

3. Scientific Foundations

3.1. Structure-preserving numerical schemes for solving ordinary differential equations

Keywords: *Hamiltonian system, Lie-group system, invariant, numerical integrator, ordinary differential equation, reversible system.*

Participants: François Castella, Philippe Chartier, Erwan Faou.

In many physical situations, the time-evolution of certain quantities may be written as a Cauchy problem for a differential equation of the form

$$\begin{aligned} y'(t) &= f(y(t)), \\ y(0) &= y_0. \end{aligned} \tag{1}$$

For a given y_0 , the solution $y(t)$ at time t is denoted $\phi_t(y_0)$. For fixed t , ϕ_t becomes a function of y_0 called the *flow* of (1). From this point of view, a numerical scheme with step size h for solving (1) may be regarded as an approximation Φ_h of ϕ_h . One of the main questions of *geometric integration* is whether *intrinsic* properties of ϕ_t may be passed on to Φ_h .

This question can be more specifically addressed in the following situations:

3.1.1. Reversible ODEs

The system (1) is said to be ρ -reversible if there exists an involutive linear map ρ such that

$$\rho \circ \phi_t = \phi_t^{-1} \circ \rho = \phi_{-t} \circ \rho. \tag{2}$$

It is then natural to require that Φ_h satisfies the same relation. If this is so, Φ_h is said to be *symmetric*. Symmetric methods for reversible systems of ODEs are just as much important as *symplectic* methods for Hamiltonian systems and offer an interesting alternative to symplectic methods.

3.1.2. ODEs with an invariant manifold

The system (1) is said to have an invariant manifold g whenever

$$\mathcal{M} = \{y \in \mathbb{R}^n; g(y) = 0\} \quad (3)$$

is kept *globally* invariant by ϕ_t . In terms of derivatives and for sufficiently differentiable functions f and g , this means that

$$\forall y \in \mathcal{M}, g'(y)f(y) = 0.$$

As an example, we mention Lie-group equations, for which the manifold has an additional group structure. This could possibly be exploited for the space-discretisation. Numerical methods amenable to this sort of problems have been reviewed in a recent paper [25] and divided into two classes, according to whether they use g explicitly or through a projection step. In both cases, the numerical solution is forced to live on the manifold at the expense of some Newton's iterations.

3.1.3. Hamiltonian systems

Hamiltonian problems are ordinary differential equations of the form:

$$\begin{aligned} \dot{p}(t) &= -\nabla_q H(p(t), q(t)) \in \mathbb{R}^d \\ \dot{q}(t) &= \nabla_p H(p(t), q(t)) \in \mathbb{R}^d \end{aligned} \quad (4)$$

with some prescribed initial values $(p(0), q(0)) = (p_0, q_0)$ and for some scalar function H , called the Hamiltonian. In this situation, H is an invariant of the problem. The evolution equation (4) can thus be regarded as a differential equation on the manifold

$$\mathcal{M} = \{(p, q) \in \mathbb{R}^d \times \mathbb{R}^d; H(p, q) = H(p_0, q_0)\}.$$

Besides the Hamiltonian function, there might exist other invariants for such systems: when there exist d invariants in involution, the system (4) is said to be *integrable*. Consider now the parallelogram P originating from the point $(p, q) \in \mathbb{R}^{2d}$ and spanned by the two vectors $\xi \in \mathbb{R}^{2d}$ and $\eta \in \mathbb{R}^{2d}$, and let $\omega(\xi, \eta)$ be the sum of the *oriented* areas of the projections over the planes (p_i, q_i) of P ,

$$\omega(\xi, \eta) = \xi^T J \eta,$$

where J is the *canonical symplectic* matrix

$$J = \begin{bmatrix} 0 & I_d \\ -I_d & 0 \end{bmatrix}.$$

A continuously differentiable map g from \mathbb{R}^{2d} to itself is called *symplectic* if it preserves ω , i.e. if

$$\omega(g'(p, q)\xi, g'(p, q)\eta) = \omega(\xi, \eta).$$

A fundamental property of Hamiltonian systems is that their exact flow is symplectic. Integrable Hamiltonian systems behave in a very remarkable way: as a matter of fact, their invariants persist under small perturbations, as shown in the celebrated theory of Kolmogorov, Arnold and Moser. This behavior motivates the introduction of *symplectic* numerical flows that share most of the properties of the exact flow. For practical simulations of Hamiltonian systems, symplectic methods possess an important advantage: the error-growth as a function of time is indeed linear, whereas it would typically be quadratic for non-symplectic methods.

3.1.4. Differential-algebraic equations

Whenever the number of differential equations is insufficient to determine the solution of the system, it may become necessary to solve the differential part and the constraint part altogether. Systems of this sort are called differential-algebraic systems. They can be classified according to their index, yet for the purpose of this expository section, it is enough to present the so-called index-2 systems

$$\begin{aligned} \dot{y}(t) &= f(y(t), z(t)), \\ 0 &= g(y(t)), \end{aligned} \quad (5)$$

where initial values $(y(0), z(0)) = (y_0, z_0)$ are given and assumed to be consistent with the constraint manifold. By constraint manifold, we imply the intersection of the manifold

$$\mathcal{M}_1 = \{y \in \mathbb{R}^n, g(y) = 0\}$$

and of the so-called hidden manifold

$$\mathcal{M}_2 = \{(y, z) \in \mathbb{R}^n \times \mathbb{R}^m, \frac{\partial g}{\partial y}(y) f(y, z) = 0\}.$$

This manifold $\mathcal{M} = \mathcal{M}_1 \cap \mathcal{M}_2$ is the manifold on which the exact solution $(y(t), z(t))$ of (5) lives.

There exists a whole set of schemes which provide a numerical approximation lying on \mathcal{M}_1 . Furthermore, this solution can be projected on the manifold \mathcal{M} by standard projection techniques. However, it is worth mentioning that a projection destroys the symmetry of the underlying scheme, so that the construction of a symmetric numerical scheme preserving \mathcal{M} requires a more sophisticated approach.

3.2. Highly-oscillatory systems

Keywords: *oscillatory solutions, second-order ODEs, step size restrictions.*

Participants: François Castella, Philippe Chartier, Erwan Faou.

In applications to molecular dynamics or quantum dynamics for instance, the right-hand side of (1) involves *fast* forces (short-range interactions) and *slow* forces (long-range interactions). Since *fast* forces are much cheaper to evaluate than *slow* forces, it seems highly desirable to design numerical methods for which the number of evaluations of slow forces is not (at least not too much) affected by the presence of fast forces.

A typical model of highly-oscillatory systems is the second-order differential equations

$$\ddot{q} = -\nabla V(q) \quad (6)$$

where the potential $V(q)$ is a sum of potentials $V = W + U$ acting on different time-scales, with $\nabla^2 W$ positive definite and $\|\nabla^2 W\| \gg \|\nabla^2 U\|$. In order to get a bounded error propagation in the linearized equations for an explicit numerical method, the step size must be restricted according to

$$h\omega < C,$$

where C is a constant depending on the numerical method and where ω is the highest frequency of the problem, i.e. in this situation the square root of the largest eigenvalue of $\nabla^2 W$. In applications to molecular dynamics for instance, *fast* forces deriving from W (short-range interactions) are much cheaper to evaluate than *slow* forces deriving from U (long-range interactions). In this case, it thus seems highly desirable to design numerical methods for which the number of evaluations of slow forces is not (at least not too much) affected by the presence of fast forces.

Another prominent example of highly-oscillatory systems is encountered in quantum dynamics where the Schrödinger equation is the model to be used. Assuming that the Laplacian has been discretized in space, one indeed gets the *time*-dependent Schrödinger equation:

$$i\dot{\psi}(t) = \frac{1}{\varepsilon}H(t)\psi(t), \quad (7)$$

where $H(t)$ is finite-dimensional matrix and where ε typically is the square-root of a mass-ratio (say electron/ion for instance) and is small ($\varepsilon \approx 10^{-2}$ or smaller). Through the coupling with classical mechanics ($H(t)$ is obtained by solving some equations from classical mechanics), we are confronted once again to two different time-scales, 1 and ε . In this situation also, it is thus desirable to devise a numerical method able to advance the solution by a time-step $h > \varepsilon$.

3.3. Geometric schemes for the Schrödinger equation

Keywords: *Schrödinger equation, energy conservation, variational splitting.*

Participants: François Castella, Philippe Chartier, Erwan Faou.

Given the Hamiltonian structure of the Schrödinger equation, we are led to consider the question of energy preservation for time-discretization schemes.

At a higher level, the Schrödinger equation is a partial differential equation which may exhibit Hamiltonian structures. This is the case of the time-dependent Schrödinger equation, which we may write as

$$i\varepsilon \frac{\partial \psi}{\partial t} = H\psi, \quad (8)$$

where $\psi = \psi(x, t)$ is the wave function depending on the spatial variables $x = (x_1, \dots, x_N)$ with $x_k \in \mathbb{R}^d$ (e.g., with $d = 1$ or 3 in the partition) and the time $t \in \mathbb{R}$. Here, ε is a (small) positive number representing the scaled Planck constant and i is the complex imaginary unit. The Hamiltonian operator H is written

$$H = T + V$$

with the kinetic and potential energy operators

$$T = - \sum_{k=1}^N \frac{\varepsilon^2}{2m_k} \Delta_{x_k} \quad \text{and} \quad V = V(x),$$

where $m_k > 0$ is a particle mass and Δ_{x_k} the Laplacian in the variable $x_k \in \mathbb{R}^d$, and where the real-valued potential V acts as a multiplication operator on ψ .

The multiplication by i in (8) plays the role of the multiplication by J in classical mechanics, and the energy $\langle \psi | H | \psi \rangle$ is conserved along the solution of (8), using the physicists' notations $\langle u | A | u \rangle = \langle u, Au \rangle$ where $\langle \cdot, \cdot \rangle$ denotes the Hermitian L^2 -product over the phase space. In quantum mechanics, the number N of particles is very large making the direct approximation of (8) very difficult.

The numerical approximation of (8) can be obtained using projections onto submanifolds of the phase space, leading to various PDEs or ODEs: see [30][31] for reviews, and [23] for the case of Gaussian wave packets dynamics detailed in Section 5.4. However the long-time behavior of these approximated solutions is well understood only in this latter case, where the dynamics turns out to be finite dimensional. In the general case, it is very difficult to prove the preservation of qualitative properties of (8) such as energy conservation or growth in time of Sobolev norms. The reason for this is that backward error analysis is not directly applicable for PDEs. Overwhelming these difficulties is thus a very interesting challenge.

A particularly interesting case of study is given by symmetric splitting methods, such as the Strang splitting:

$$\psi_1 = \exp(-i(\delta t)V/2) \exp(i(\delta t)\Delta) \exp(-i(\delta t)V/2) \psi_0 \quad (9)$$

where δt is the time increment (we have set all the parameters to 1 in the equation). As the Laplace operator is unbounded, we cannot apply the standard methods used in ODEs to derive long-time properties of these schemes. However, its projection onto finite dimensional submanifolds (such as Gaussian wave packets space

or FEM finite dimensional space of functions in x) may exhibit Hamiltonian or Poisson structure, whose long-time properties turn out to be more tractable.

3.4. High-frequency limit of the Helmholtz equation

Keywords: *Helmholtz equation, high oscillations, waves.*

Participant: François Castella.

The Helmholtz equation modelizes the propagation of waves in a medium with variable refraction index. It is a simplified version of the Maxwell system for electro-magnetic waves.

The high-frequency regime is characterized by the fact that the typical wavelength of the signals under consideration is much smaller than the typical distance of observation of those signals. Hence, in the high-frequency regime, the Helmholtz equation at once involves highly oscillatory phenomena that are to be described in some asymptotic way. Quantitatively, the Helmholtz equation reads

$$i\alpha_\varepsilon u_\varepsilon(x) + \varepsilon^2 \Delta_x u_\varepsilon + n^2(x)u_\varepsilon = f_\varepsilon(x).$$

Here, ε is the small adimensional parameter that measures the typical wavelength of the signal, $n(x)$ is the space-dependent refraction index, and $f_\varepsilon(x)$ is a given (possibly dependent on ε) source term. The unknown is $u_\varepsilon(x)$. One may think of an antenna emitting waves in the whole space (this is the $f_\varepsilon(x)$), thus creating at any point x the signal $u_\varepsilon(x)$ along the propagation. The small $\alpha_\varepsilon > 0$ term takes into account damping of the waves as they propagate.

One important scientific objective typically is to describe the high-frequency regime in terms of *rays* propagating in the medium, that are possibly refracted at interfaces, or bounce on boundaries, etc. Ultimately, one would like to replace the true numerical resolution of the Helmholtz equation by that of a simpler, asymptotic model, formulated in terms of rays.

In some sense, and in comparison with, say, the wave equation, the specificity of the Helmholtz equation is the following. While the wave equation typically describes the evolution of waves between some initial time and some given observation time, the Helmholtz equation takes into account at once the propagation of waves over *infinitely long* time intervals. Qualitatively, in order to have a good understanding of the signal observed in some bounded region of space, one readily needs to be able to describe the propagative phenomena in the whole space, up to infinity. In other words, the “rays” we refer to above need to be understood from the initial time up to infinity. This is a central difficulty in the analysis of the high-frequency behaviour of the Helmholtz equation.

3.5. From the Schrödinger equation to Boltzmann-like equations

Keywords: *Boltzmann equation, Schrödinger equation, asymptotic model.*

Participant: François Castella.

The Schrödinger equation is the appropriate to describe transport phenomena at the scale of electrons. However, for real devices, it is important to derive models valid at a larger scale.

In semi-conductors, the Schrödinger equation is the ultimate model that allows to obtain quantitative information about electronic transport in crystals. It reads, in convenient adimensional units,

$$i\partial_t \psi(t, x) = -\frac{1}{2} \Delta_x \psi + V(x)\psi,$$

where $V(x)$ is the potential and $\psi(t, x)$ is the time- and space-dependent wave function. However, the size of real devices makes it important to derive simplified models that are valid at a larger scale. Typically, one wishes to have kinetic transport equations. As is well-known, this requirement needs one to be able to describe “collisions” between electrons in these devices, a concept that makes sense at the macroscopic level, while it does not at the microscopic (electronic) level. Quantitatively, the question is the following: can one obtain the Boltzmann equation (an equation that describes collisional phenomena) as an asymptotic model for the

Schrödinger equation, along the physically relevant micro-macro asymptotics? From the point of view of modelling, one wishes here to understand what are the “good objects”, or, in more technical words, what are the relevant “cross-sections”, that describe the elementary collisional phenomena. Quantitatively, the Boltzmann equation reads, in a simplified, linearized, form :

$$\partial_t f(t, x, v) = \int_{\mathbf{R}^3} \sigma(v, v') [f(t, x, v') - f(t, x, v)] dv'.$$

Here, the unknown is $f(x, v, t)$, the probability that a particle sits at position x , with a velocity v , at time t . Also, $\sigma(v, v')$ is called the cross-section, and it describes the probability that a particle “jumps” from velocity v to velocity v' (or the converse) after a collision process.

3.6. Spatial approximation for solving ODEs

Keywords: *manifold, spatial approximation, triangulation.*

Participants: Philippe Chartier, Erwan Faou.

The technique consists in solving an approximate initial value problem on an approximate invariant manifold for which an atlas consisting of *easily computable* charts exists. The numerical solution obtained in this way never drifts off the exact manifold considerably even for long-time integration.

Instead of solving the initial Cauchy problem, the technique consists in solving an approximate initial value problem of the form:

$$\begin{aligned} \tilde{y}'(t) &= \tilde{f}(\tilde{y}(t)), \\ \tilde{y}(0) &= \tilde{y}_0, \end{aligned} \tag{10}$$

on an invariant manifold $\tilde{\mathcal{M}} = \{y \in \mathbb{R}^n; \tilde{g}(y) = 0\}$, where \tilde{f} and \tilde{g} approximate f and g in a sense that remains to be defined. The idea behind this approximation is to replace the differential manifold \mathcal{M} by a suitable approximation $\tilde{\mathcal{M}}$ for which an atlas consisting of *easily computable* charts exists. If this is the case, one can reformulate the vector field \tilde{f} on each domain of the atlas in an *easy* way. The main obstacle of *parametrization* methods [32] or of *Lie-methods* [29] is then overcome.

The numerical solution obtained in this way obviously does not lie on the exact manifold: it lives on the approximate manifold $\tilde{\mathcal{M}}$. Nevertheless, it never drifts off the exact manifold considerably, if \mathcal{M} and $\tilde{\mathcal{M}}$ are chosen appropriately *close* to each other.

An obvious prerequisite for this idea to make sense is the existence of a neighborhood \mathcal{V} of \mathcal{M} containing the approximate manifold $\tilde{\mathcal{M}}$ and on which the vector field f is well-defined. In contrast, if this assumption is fulfilled, then it is possible to construct a new admissible vector field \tilde{f} given \tilde{g} . By admissible, we mean tangent to the manifold $\tilde{\mathcal{M}}$, i.e. such that

$$\forall y \in \tilde{\mathcal{M}}, \tilde{G}(y)\tilde{f}(y) = 0,$$

where, for convenience, we have denoted $\tilde{G}(y) = \tilde{g}'(y)$. For any $y \in \tilde{\mathcal{M}}$, we can indeed define

$$\tilde{f}(y) = (I - P(y))f(y), \tag{11}$$

where $P(y) = \tilde{G}^T(y)(\tilde{G}(y)\tilde{G}^T(y))^{-1}\tilde{G}(y)$ is the projection along $\tilde{\mathcal{M}}$.

4. Application Domains

4.1. Laser physics

Laser physics considers the propagation over long space (or time) scales of high frequency waves. Typically, one has to deal with the propagation of a wave having a wavelength of the order of $10^{-6}m$, over distances of the order $10^{-2}m$ to 10^4m . In these situations, the propagation produces both a short-scale oscillation and

exhibits a long term trend (drift, dispersion, nonlinear interaction with the medium, or so), which contains the physically important feature. For this reason, one needs to develop ways of filtering the irrelevant high-oscillations, and to build up models and/or numerical schemes that do give information on the long-term behavior. In other terms, one needs to develop high-frequency models and/or high-frequency schemes.

This task has been partially performed in the context of a contract with Alcatel, in that we developed a new numerical scheme to discretize directly the high-frequency model derived from physical laws.

Generally speaking, the demand in developing such models or schemes in the context of laser physics, or laser/matter interaction, is large. It involves both modeling and numerics (description of oscillations, structure preserving algorithms to capture the long-time behaviour, etc).

In a very similar spirit, but at a different level of modelling, one would like to understand the very coupling between a laser propagating in, say, a fiber, and the atoms that build up the fiber itself.

The standard, quantum, model in this direction is called the Bloch model: it is a Schrödinger like equation that describes the evolution of the atoms, when coupled to the laser field. Here the laser field induces a potential that acts directly on the atom, and the link between this potential and the laser itself is given by the so-called dipolar matrix, a matrix made up of physical coefficients that describe the polarization of the atom under the applied field.

The scientific objective here is twofold. First, one wishes to obtain tractable asymptotic models that average out the high oscillations of the atomic system and of the laser's field. A typical phenomenon here is the *resonance* between the field and the energy levels of the atomic system. Second, one wishes to obtain good numerical schemes in order to solve the Bloch equation, beyond the oscillatory phenomena entailed by this model.

4.2. Molecular Dynamics

In classical molecular dynamics, the equations describe the evolution of atoms or molecules under the action of forces deriving from several interaction potentials. These potentials may be short-range or long-range and are treated differently in most molecular simulation codes. In fact, long-range potentials are computed at only a fraction of the number of steps. By doing so, one replaces the vector field by an approximate one and alternates steps with the exact field and steps with the approximate one. Although such methods have been known and used with success for years, very little is known on how the "space" approximation (of the vector field) and the time discretization should be combined in order to optimize the convergence. Also, the fraction of steps where the exact field is used for the computation is mainly determined by heuristic reasons and a more precise analysis seems necessary. Finally, let us mention that similar questions arise when dealing with constrained differential equations, which are a by-product of many simplified models in molecular dynamics (this is the case for instance if one replaces the highly-oscillatory components by constraints).

5. New Results

5.1. Long-time averages for molecular simulations

Participants: Francois Castella, Philippe Chartier, Erwan Faou.

Given a Hamiltonian dynamics of the form (4), it is a common problem (for instance in molecular dynamics simulations) to estimate the *space* average of an observable A over a manifold S (say a surface of constant energy for instance)

$$\langle A \rangle := \int_S A(q, p) d\sigma(q, p), \quad (12)$$

through the limit of the *time* average

$$\langle A \rangle(T) := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T A(q(t), p(t)) dt. \quad (13)$$

The conditions under which the two quantities coincide are not known in general and this is a difficult and largely open question linked to the *ergodicity* of the system. In contrast, if the Hamiltonian system is assumed to be *integrable*, a well-known result states that, under a *diophantine* condition, the time-average converges to its space-counterpart with a rate of $1/T$.

In a first step, in collaboration with the INRIA-team MICMAC of the Ecole Nationale des Ponts et Chaussées, we have shown that the convergence of the *time average* (13) toward the *space average* (12) can be accelerated through the use of weighted integrals of the form

$$\int_0^T \phi\left(\frac{t}{T}\right) A(q(t), p(t)) dt, \quad (14)$$

where ϕ is a *filter* function. This has led us to the definition of a close-to-optimal filter which brings a significant speed-up. To become of practical use, the integrals involved in the averages need to be discretized and evaluated not along the exact trajectory, which is obviously not available, but along a numerical approximation of it. In this context, symplectic integrators naturally come into play, since the length T of the interval of integration is allowed to become “as large as necessary” for the convergence to occur. The use of some basic symplectic schemes in combination with filtered averages define a practical method, which, in some physically relevant situations, has proven to be a real improvement over the usual averaging technique, as demonstrated by numerical experiments.

5.2. Constrained Hamiltonian systems and differential-algebraic systems

Participant: Philippe Chartier.

Constrained Hamiltonian systems with holonomic constraints (i.e. constraints involving only the positions) appear typically when dissipative forces (such as *friction*) may be neglected. In this situation, a Lagrange-type principle allows to write the equations of the dynamics as

$$\begin{aligned} p' &= -\nabla_q H - \lambda^T C(q) \\ q' &= \nabla_p H, \\ 0 &= c(q) \end{aligned} \quad (15)$$

where, when compared to (4), the additional terms λ , $c(q)$ and $C(q)$ denote respectively the Lagrange multipliers, the function of constraints and its first derivative. As in (4), the exact flow is symplectic and preserves the Hamiltonian. A prominent example (as a toy-problem) of such systems is the *double-pendulum*, a system composed of two connected arms moving below its fixed point without friction in the field of gravity. However, this is just one of the numerous more complex systems encountered in robotics. Notice eventually, that as a DAE, problem (15) is usually of index 3.

An ideal numerical method for (15) would preserve the constraints, the two hidden constraints obtained by differentiation, the Hamiltonian function and the symplecticity of the flow. The Lobatto IIIA-III B pair is very appealing, since it is both symplectic and preserves the constraints. However, it has some limitations regarding stability for stiff systems.

An alternative approach consists in differentiating once the constraints c and solving the resulting index-2 system. This technique is usually dismissed, in particular for long-term integration, for there are no symplectic methods for the index-2 formulation, but the situation is completely changed if the system is *reversible*, i.e. if there exist isomorphisms ρ and $\tilde{\rho}$ such that the functions f and g of (5) satisfy

$$\rho f(y, z) = -f(\rho y, z) \quad \text{and} \quad g(\rho y) = \tilde{\rho} g(y). \quad (16)$$

We have shown in [15] that symmetric Runge-Kutta together with a suitable *symmetric projection* procedure mimic the qualitative behavior of Hamiltonian systems with holonomic constraints.

5.3. A Poisson system with boundary conditions

Participants: François Castella, Philippe Chartier, Erwan Faou.

This work is related to the contract with Alcatel (see Section 6.1) and is devoted to the mathematical and numerical aspects of a model for a n -th order cascaded Raman device. In their discretized version, the equations involve waves traveling backward and forward in the cavity, and interacting together via the Raman gain. Let us briefly present the most significant aspects of the Alcatel model with geometric integration in view: denote by L the length of the cavity, and suppose that n rays at given frequencies $\nu_1, \nu_2, \dots, \nu_n$ are represented by $2n$ functions $F_i(x)$ and $B_i(x)$ for $x \in (0, L)$ denoting the powers of the *forward* and *backward* waves respectively.

The model equations can now be written as follows, where the index i runs from 0 to n :

$$\begin{aligned}\dot{F}_i &= -\alpha_i F_i - \sum_{j < i} g_{ij} (F_j + B_j) F_i + \sum_{j > i} g_{ij} (F_j + B_j) F_i, \\ \dot{B}_i &= \alpha_i B_i + \sum_{j < i} g_{ij} (F_j + B_j) B_i - \sum_{j > i} g_{ij} (F_j + B_j) B_i.\end{aligned}\quad (17)$$

The coefficients g_{ij} are non-negative and represent the Raman gain between the wave length of the level i and j . The coefficients $\alpha_i > 0$ are attenuation coefficients.

It is interesting to notice that the system has several mathematical invariants. A simple calculation shows indeed that

$$\forall i = 1, \dots, n, \quad \forall x \in (0, L), \quad (F_i B_i)(x) = (F_i B_i)(0) = (F_i B_i)(L).$$

If we make the further assumption that the exchange of energy is symmetric through the Raman process, and that there is no loss of energy within the fiber, then we can further notice that $\sum_j (F_j - B_j)$ is kept constant along the fiber. This quantity can be interpreted as the energy of the system and its preservation in absence of attenuation is physically sounded.

The existence of these two invariants becomes natural if one notices that the ODE system (17) has a Poisson structure (i.e. a Hamiltonian-type structure where the canonical matrix J in (4) is replaced by a suitable matrix B depending on the point (p, q)). It is a well-know fact that such systems can be brought back to canonical form, through a local change of variables. In the context of the present study, it is in fact possible to exhibit a *global* change of variables, whose existence is of main importance to devise the algorithm implemented for Alcatel [14].

More recently, the collaboration with Alcatel has given rise to the following new question: while the above model describes in a reasonable way the so-called Self-Phase-Modulation (SPM), and the Cross-Phase-Modulation (XPM) effects, it does not take into account the so-called Four-Wave-Mixing (FWM). Is it possible to modify the model in order to encode FWM ?

Let us be more precise. The above model is a high-frequency model that is asymptotic to the Maxwell system. Here, the nonlinear terms stem from cubic nonlinearities at the Maxwell level, that encode the reaction of the fiber to the applied laser field. In that picture, FWM terms correspond to nonlinear terms that have been neglected in the asymptotic process leading from Maxwell's equations to the above Lotka-Volterra like model. The question is thus to recover those neglected terms upon making a refined asymptotic analysis that takes into account the true physical orders of magnitude of the various phenomena.

5.4. Gaussian wave packets

Participant: Erwan Faou.

The work described in this section has been conducted in collaboration with Chr. Lubich, from the University of Tübingen (Germany).

Gaussian wavepacket dynamics is widely used in quantum molecular dynamics, see for instance [28][24]. In this case, an approximation to the wave function $\psi(x, t)$ solution of (8) is sought for in the form

$$u(x, t) = e^{i\varphi(t)/\varepsilon} \prod_{k=1}^N \phi_k(x_k, t) \quad (18)$$

with

$$\phi_k(x_k, t) = \exp\left(\frac{i}{\varepsilon} (a_k(t) |x_k - q_k(t)|^2 + p_k(t) \cdot (x_k - q_k(t)) + c_k(t)\right), \quad (19)$$

where $|\cdot|$ and \cdot denote the Euclidean norm and inner product on \mathbb{R}^d , respectively. The parameters $q_k \in \mathbb{R}^d$ and $p_k \in \mathbb{R}^d$ represent the position and momentum average, respectively: $q_k = \langle u | x_k | u \rangle$ and $p_k = \langle u | -i\varepsilon \nabla_{x_k} | u \rangle$. Further, $a_k = \alpha_k + i\beta_k$ (with $\beta_k > 0$) is a complex width parameter, $c_k = \gamma_k + i\delta_k$ is a complex phase parameter, and φ is a real phase. (Only the sum of the phases $\varphi + \sum_k c_k$ is determined uniquely. The partition of the phases is made by convenience so that each ϕ_k is of unit norm.)

The Dirac-Frenkel-McLachlan variational principle yields equations of motion for these parameters. It turns out that this system of ordinary differential equations has a Poisson structure inherited from the Hamiltonian structure of the Schrödinger equation, and that to the semi-classical limit $\varepsilon \rightarrow 0$, these equations tends to the finite dimensional Hamiltonian system $\dot{q}_k = p_k/m_k, \dot{p}_k = -\nabla_{q_k} V(q)$.

In [23], C. Lubich and E. Faou show that the projection of the splitting scheme (9) onto the sub-manifold made of Gaussian wave packets yields a numerical scheme that is a Poisson integrator, which can be computed explicitly. Using backward error analysis, this shows in particular the conservation of energy for exponentially long time. If the potential has a rotational symmetry so that the angular momentum is conserved in the full quantum dynamics, then the numerical integrator also preserves the angular momentum.

In the classical limit $\varepsilon \rightarrow 0$, the position and momentum approximations q_k^n, p_k^n converge to the position and momentum approximations obtained by applying the Störmer-Verlet method to the classical limit system $\dot{q}_k = p_k/m_k, \dot{p}_k = -\nabla_{q_k} V(q)$.

5.5. Energy conservation

Participant: Erwan Faou.

This work has been made in collaboration with E. Hairer and T.-L. Pham (University of Geneva). We consider the numerical solution of Hamiltonian systems

$$\begin{aligned} \dot{p} &= -\nabla_q H(p, q) \\ \dot{q} &= \nabla_p H(p, q) \end{aligned} \quad \text{or} \quad \dot{y} = J^{-1} \nabla H(y), \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \quad (20)$$

where $y = (p, q)^T$ and $H(y) = H(p, q)$ is a real-valued smooth function. Since J is skew-symmetric, the Hamiltonian $H(y)$ is a first integral of the system.

For a numerical integration it is of interest to know whether the Hamiltonian remains also constant or nearly constant along the numerical solution over very long time intervals. It is known (see [26] for a review) that symplectic one-step methods nearly conserve the Hamiltonian of an arbitrary system (20) over exponentially long times. This conservation still holds in the case of symmetric multistep methods applied to Hamiltonian systems of the form $H(p, q) = \frac{1}{2}p^T p + U(q)$. Moreover, if the system is integrable and reversible, symmetric reversible one-step methods nearly conserve all action variables of a reversible integrable system. In many other situations it is observed that the numerical solution also well conserves the Hamiltonian over long times but a theoretical explanation is missing.

In [18], E. Faou, E. Hairer and T.-L. Pham show that the energy conservation relies on conditions on the coefficients of the method, and that if these conditions are not satisfied, we can exhibit counter-examples showing that not all symmetric Runge-Kutta methods nearly conserve the Hamiltonian even if (20) is reversible with respect to the reflection $p \longleftrightarrow -p$.

5.6. From the Bloch model to the rate equations

Participant: François Castella.

In references [10] and [11], we study the reaction of an atomic system under an applied laser field. The original equation is the above mentioned Bloch model, a Schrödinger like equation, and the laser field then

takes the form of a highly oscillatory forcing in the equation. Here, the dominant phenomenon lies in the resonant interaction between the oscillatory modes of the field and the natural oscillatory modes (= energy levels) of the atom itself.

Following the physical literature, we prove in this paper that this coupling is asymptotically described by a so-called rate equation, i.e. a linear Boltzmann equation. It describes the transitions of the electronic cloud between the atom's energy levels, as they are induced by the laser's forcing. The main difficulty in this analysis lies in the averaging out of high-oscillations, together with the sorting out of the "resonances" in the model.

5.7. From the Schrödinger to the Boltzmann equation

Participant: François Castella.

In references [9][20], we study the behavior of a system made up of a large number N of electrons. These electrons are all coupled through a given potential. This is a simplified version of a gas of electrons as it may be encountered in true semi-conductor devices. Following the physically relevant orders of magnitude, we study this system over large time intervals, and when the coupling is weak. It is well known in the semi-conductor-physics literature that such a situation is well described, asymptotically, by a nonlinear Boltzmann equation.

In Ref. [9], we give a partial result that indeed establishes the convergence of the original Schrödinger equation toward the nonlinear Boltzmann equation. In Ref. [20], we study the case when the fermionic behaviour of the electrons is taken into account, i.e. when the Pauli exclusion principle is used. We compute the associated corrective terms in the limiting Boltzmann equation.

5.8. High frequency limit of the Helmholtz equation

Participant: François Castella.

In Ref. [13], we study the so-called radiation condition at infinity in the high-frequency Helmholtz equation. This leads us to a very precise analysis of the geometric features of wave propagation in a medium with variable refraction index. In some sense, we prove that, if the refraction index is such that the rays are not captured in bounded regions of space, then the Sommerfeld radiation condition at infinity is a reasonable boundary condition along the high-frequency process. This criterion is shown to be "optimal" in that rays captured in bounded regions do provide anomalous propagative phenomena that rule out the Sommerfeld radiation condition. We use here a wave packets approach, in a similar spirit as in [23].

5.9. An algebraic approach to invariant preserving integrators

Participants: Philippe Chartier, Erwan Faou.

Given a system of differential equations (1), a B-series $B(\alpha)$ is a formal expression of the form

$$B(\alpha) = id_{\mathbb{R}^n} + \sum_{t \in \mathcal{T}} \frac{h^{|t|}}{\sigma(t)} a(t) F(t) \quad (21)$$

where the index set \mathcal{T} is the set of rooted trees, $|\cdot|$, σ and F are real functions defined on \mathcal{T} , and where a is a function defined on \mathcal{T} as well which characterizes the B-series itself. In this work, conducted in collaboration with A. Murua from the University of Basque Country, we provide algebraic conditions for the preservation of general invariants (quadratic, polynomial or Hamiltonian) by numerical methods which can be written as B-series. The existence of a modified invariant is also investigated and turns out to be equivalent, up to a conjugation, to the preservation of the exact invariant. A striking corollary is that a *symplectic* method is formally conjugate to a method that preserves the Hamiltonian exactly. Another surprising consequence is that the underlying one-step method of a symmetric multistep scheme is formally conjugate to a canonical B-series when applied to Newton's equations of motion.

To be more specific, we prove the following results:

1. a B-series integrator possesses a modified invariant for all problems with an invariant if and only if it is conjugate to the exact flow;

2. a B-series integrator possesses a modified invariant for all problems with a *quadratic* invariant if and only if it is conjugate to a *symplectic* method;
3. a B-series integrator possesses a modified Hamiltonian for all *Hamiltonian* problems if and only if it is conjugate to a method that preserves the Hamiltonian exactly;
4. a symplectic B-series is formally conjugate to a B-series that preserves the Hamiltonian exactly.

The corresponding paper [22] is about to be submitted and is currently available at <http://www.irisa.fr/ipso/perso/chartier/#publications>

5.10. Shell theory

Participant: Erwan Faou.

The paper *Multiscale expansions for linear clamped elliptic shells* [17] has been accepted for publication in Communication in Partial Differential Equations. This paper corresponds to the second part of E. Faou's Thesis.

In collaboration with M. Dauge (CNRS - University of Rennes 1) and Z. Yosibash (Beer Sheva - Israël), E. Faou wrote the chapter 8, Volume I of the Encyclopedia for Computational Mechanics published in 2004, and edited by Erwin Stein, René de Borst and Thomas J.R. Hughes, [16]. This chapter is a survey of recent works on plates and shells. We develop and explain theoretical results, derive new results in the direction of hierarchical models and eventually give new numerical experiments concerning the eigenmodes of shells in the very interesting case of sensitive shells, where no standard multiscale expansion technics apply.

5.11. Spatial approximation for solving ODEs

Participants: Philippe Chartier, Erwan Faou.

We are concerned here with numerical methods which combine spatial and time discretization in order to increase the stability, or to respect the features of the problem up to a prescribed tolerance. At this point, we would like to point out the specificity of our approach, for most existing methods either strictly respect the manifold or embed a drift that goes out of control with increasing time. The methods we are concerned with rely on an "a-priori" spatial approximation of the manifold with a specified error, together with a time-approximation that preserves exactly this approximate manifold. The distance of the numerical solution to the exact manifold is thus expected to remain bounded, even for infinite times if the manifold is compact. It has probably become clear to the reader that other structural properties of the exact solution, such as symplecticity or symmetry, will impose restrictions both on the space-discretization and on the time-discretization that we are willing to combine.

The question of the computational cost of this a-priori discretization of the manifold has to be addressed: at present, the performances of the various existing methods for solving one and only one trajectory seem out of reach. However, the positions are reversed if many trajectories need to be computed. It may also be the case that the vector field is not known on the whole set of definition of the equations, in which case some "reconstruction" of it is anyway necessary. We will thus focus on applications which belong to at least one of the two categories.

The first schemes we propose rely on the following construction:

- The phase space (i.e. the invariant manifold) $\tilde{\mathcal{M}}$ is triangulated as

$$\tilde{\mathcal{M}} = \bigcup_{j \in J} K_j, \quad (22)$$

where the K_j 's are compact connected domains with piecewise smooth boundaries ∂K_j and J is countable set of indices. Note that we will mainly consider the cases where the K_j 's are hyper-triangles or hypercubes.

- On each domain K_j an approximation \tilde{f}_j of f is known of a given order k independent of j , that is to say

$$\|\tilde{f}_j - f\|_{K_j} \leq C\tau^k, \quad (23)$$

where τ is a characteristic dimension of the triangulation and C a positive constant independent of j .

If we approximate the solution of the initial value problem (1) on each domain K_j by a p -th order one-step method, then an error bound of the form

$$\|E(T)\| \leq C(T)(\tau^k + h^p)$$

can be obtained, where h denotes the maximum step-size used for the time integration and $E(T)$ the global error of the solution at time T . Based on this somehow usual convergence analysis, we can elaborate a first-order method of Euler type, for first-order approximations of the vector field, or various second-order schemes for affine approximations of the vector field. Something very noticeable in these methods is the a-posteriori determination of the time. As a matter of fact, since the approximate manifold is defined in terms of local charts on the K_j 's, the representation of \tilde{f} has to be changed whenever the numerical solution leaves an element of the triangulation. This makes necessary to determine the exit time, i.e. the time necessary for a trajectory with initial value in K_j or on the boundary of K_j to leave K_j (note that even in the case where the manifold is simply \mathbb{R}^m , it might be highly beneficial to resort to the same technique in order to use a high-order numerical method on each K_j , since the global degree of smoothness of the approximation \tilde{f} of f may be much lower than the degree of smoothness of the \tilde{f}_j 's). Once the trajectory has left K_j , it enters a new element K_l of the triangulation and it can be advanced in time using the corresponding approximation \tilde{f}_l of f . As a consequence, the sequence of times at which approximations of the solution are computed partly depends on the space discretization.

Note that whenever the function f is ρ -reversible, i.e. such that $f \circ \rho = -\rho \circ f$ for a reflexive ρ , and if the triangulation respects this property, one may build symmetric schemes in the same way.

First results with numerical schemes of this kind will be reported soon in a forthcoming publication.

6. Contracts and Grants with Industry

Participants: Francois Castella, Philippe Chartier, Erwan Faou.

Alcatel contract.

partners : INRIA, Alcatel CIT

time : from December 2003 until December 2004.

The results presented in this section have been obtained jointly with the engineers from the laboratory of optonics from Alcatel Marcoussis. This project with Alcatel is devoted to the mathematical and numerical aspects of a model for a n -th order cascaded Raman device. In their discretized version, the equations involve waves traveling backward and forward in the cavity, and interacting together via the Raman gain. In its most general form, a n -th order cascaded Raman fiber laser is described by a set of partial differential equations. However, it has become common, based on the experience that only a few frequencies contribute significantly to the phenomenon, to discretize the full spectrum and to simulate the resulting system of ordinary differential equations. Using a change of variable, the questions of existence and uniqueness of a solution have been solved and a more efficient and more stable algorithm has been proposed and implemented [14][19]. However, this initial work has emphasized some limitations, and it now appears necessary to consider a more elaborated model, including the whole spectrum of frequencies. This model is currently under development and should

certainly require a different numerical technique. The end of the contract has consequently been postponed to 2005.

7. Other Grants and Activities

7.1. National Grants

Participants: François Castella, Philippe Chartier, Erwan Faou.

7.1.1. ARC PRESTISSIMO 2003-2004

The PRESTISSIMO group associates the members of *IPSO*, E. Cancès, C. Le Bris, F. Legoll and G. Turinici from the team MICMAC (Laboratoire CERMICS, Ecole Nationale des Ponts et Chaussées, Marne-La-Vallée), Gilles Zerah from the CEA and Olivier Coulaud from the INRIA-team ScAIApplix (INRIA Bordeaux). It is funded for two years onward from January 2003. Erwan Faou is its administrative manager. The main objective of the group is to share knowledge on time integrators for molecular dynamics simulation and to solve some of the theoretical and practical questions raised by long-time integration. Several results have been obtained and are about to be published [21][12].

A workshop was held in Paris in December, at the Institut Henri Poincaré : <http://msama.irisa.fr>

7.1.2. ACI Molecular Simulation 2004-2007

The ARC Prestissimo will now be continued through the newly funded ACI (Action Concertée incitative) 2004-2006 entitled “Simulation Moléculaire” and taking place within the program “Nouvelles Interfaces des Mathématiques”. This action associates 20 researchers and 8 teams :

- E. Cancès (MICMAC-CERMICS),
- Y. Achdou (Laboratoire J.L. Lions, Université Paris VI) ,
- O. Atabek (Laboratoire Photo-physique Moléculaire, Université Paris Sud Orsay),
- P. Rouchon (Centre Automatique et Systèmes, Ecole des Mines de Paris),
- G. Zerah (Service Physique de la Matière Condensée, CEA-DAM, Ile-de-France),
- A. Savin (Laboratoire de Chimie Théorique, Université Paris VI),
- M. Shoenauer (Projet TAO, INRIA),
- P. Chartier (Equipe IPSO, INRIA).

The main objective of this action is to propose new numerical schemes for the simulation of molecules, both at the atomistic scale (this was the focus of PRESTISSIMO) and at the quantum scale. The main objective of this ACI is to improve the numerical methods in many aspects of molecular simulation and at different scales : quantum, atomistic, and higher... The idea is to bring together mathematicians with various skills (PDEs/ODE, control, optimization...) and chemists and physicists in order to have the largest possible impact on applications. The kick-off meeting took place at CERMIS in october under the leadership of Claude Le Bris.

7.1.3. ACI High-frequency methods for ordinary and partial differential equations 2003-2006

The team is involved in a recently accepted ACI named “High-frequency methods for ordinary and partial differential equations”, François Castella being in charge of the project. The other partners of the action are listed below:

- Laboratoire de Modélisation et de Calcul - IMAG - CNRS UMR 5523 B.P. 53 - 38041 Grenoble Cedex 9
- Département de Mathématiques - Université des Sciences et Technologies de Lille

The main objective of this ACI is to settle a work-group dedicated to the study of high frequency methods for ordinary differential and partial differential equations. The methods we have in mind include homogeneization for PDEs, averaging for ODEs, kinetic methods and geometric optics. The idea is to share some of the techniques used in the PDE and ODE communities with possible applications to Hamiltonian systems, molecular and population dynamics, semi-conductors and laser-matter interactions.

8. Dissemination

8.1. Program committees, editorial Boards and organization of conferences

- E. Faou organizes the conference “Molecular simulation: algorithmic and mathematical aspects”, december 1-3, 2004, Institut Henri Poincaré : <http://msama.irisa.fr>.
- F. Castella is a member of the organizing committee of the GdR “GRIP” (Systèmes de Particules - leader : Th. Goudon).
- F. Castella has organized the summer school of the GDR “EAPQ” (Amplitude equations, leader : E. Lombard).
- F. Castella has organized with F. Golse (ENS Paris) the conference “Systèmes à grand nombre de particules: approches déterministes et stochastiques” in Rennes. The proceedings of this conference will be published in “Communications in Mathematical Sciences”.
- F. Castella has organized a one-day workshop on pure and applied analysis aimed at developing the collaboration between the universities of Rennes and Nantes, in Rennes.
- F. Castella is in charge, since 2001, of the weekly seminar of numerical analysis at the University of Rennes I.

8.2. INRIA and University committees

- P. Chartier is member of the Commission Personnel at INRIA-Rennes.
- E. Faou is member of commission de spécialistes, section 26, of the Ecole Normale Supérieure de Cachan.
- F. Castella is the leader of an "Action Concertée Incitative" “Jeunes chercheuses et jeunes chercheur” on *High-frequency methods for ordinary and partial differential equations*.
- F. Castella is member of the evaluation committee of the Austrian Graduate Program "Differential Equations Models in Science and Engineering” (leader : C. Schmeiser, Vienna).
- F. Castella is member of commission de spécialistes, sections 25-26-34, of the University of Lille.
- F. Castella is member of commission de spécialistes, section 26, of INSA, University of Rennes I.
- F. Castella is member of commission de spécialistes, section 26, of the Ecole Normale Supérieure de Cachan.

8.3. Teaching

- E. Faou is oral examiner at ENS Cachan Bruz (“agrégation”).
- F. Castella : "Electronic transport in semi-conductors", with B. Vinter (Thalès group), DEA “MM-SAP” of Versailles, Paris VI, and Ecole Polytechnique.
- F. Castella : "Numerical methods for hyperbolic problems", with G. Caloz (University of Rennes I), DEA of Mathematics, University of Rennes I.
- F. Castella : "Mathematical models in propagation phenomena", DESS of the University of Rennes I.

8.4. Participation in conferences

- F. Castella gave seminars at the universities of Nice, Nantes, Paris VI, ENS Paris, Bilbao, Rome, Grenoble, Bordeaux.
- F. Castella gave a plenary talk at CANUM - Obernai, France.
- F. Castella gave a talk at the conference “Equations aux dérivées Partielles” - Forges-les-eaux, France.

8.5. International exchanges

8.5.1. Visits

- E. Faou visited the University of Tübingen, Germany, for three months, at the invitation of Chr. Lubich.
- F. Castella visited Beijing, China, for two weeks at the invitation of P. Zhang. He gave a series of lectures for post-doctoral students at the Morningside center, Chinese Academy of Sciences.
- F. Castella visited the University of Heraklion, at the invitation of Th. Katsaounis.
- F. Castella visited the University of Roma “La Sapienza”, at the invitation of M. Pulvirenti.

8.5.2. Visitors

The team has invited the following persons :

- A. Murua, from the University of Basque Country, for a two-weeks visit.
- O. Rumborg, from KTH Stockholm, for a two-weeks visit.

9. Bibliography

Major publications by the team in recent years

- [1] G. ANDREIOIU, E. FAOU. *Complete asymptotics for shallow shells*, in "Asymptotic analysis", vol. 25, 2001, p. 239-270.
- [2] A. AUBRY, P. CHARTIER. *On improving the convergence of Radau IIA methods when applied to index-2 DAEs*, in "SIAM Journal on Numerical Analysis", vol. 35, n° 4, 1998, p. 1347-1367.
- [3] A. AUBRY, P. CHARTIER. *Pseudo-symplectic Runge-Kutta methods*, in "BIT", vol. 38, 1998, p. 439-461.
- [4] F. CASTELLA. *From the von Neumann equation to the Quantum Boltzmann equation in a deterministic framework*, in "J. Stat. Phys.", vol. 104-1/2, 2001, p. 387-447.
- [5] F. CASTELLA. *Propagation of space moments in the Vlasov-Poisson Equation and further results*, in "Ann. I.H.P., Anal. NonLin.", vol. 16-4, 1999, p. 503-533.
- [6] R. CHAN, P. CHARTIER, A. MURUA. *Post-projected Runge-Kutta methods for index-2 differential-algebraic equations*, in "Applied Numerical Mathematics", vol. 42, n° 1-3, 2002, p. 77-94.
- [7] M. DAUGE, I. DJURDJEVIC, E. FAOU, A. ROESSLE. *Eigenmode asymptotics in thin elastic plates*, in "J. Math. Pures Appl.", vol. 78, 1999, p. 925-954.
- [8] E. FAOU. *Elasticity on a thin shell: Formal series solution*, in "Asymptotic analysis", vol. 31, 2002, p. 317-361.

Articles in referred journals and book chapters

- [9] D. BENEDETTO, F. CASTELLA, R. ESPOSITO, M. PULVIRENTI. *Some considerations on the derivation of the nonlinear quantum Boltzmann equation*, in "J. Stat. Phys.", vol. 116-1/4, 2004, p. 381-410.
- [10] B. BIDÉGARAY, F. CASTELLA, P. DEGOND. *From Bloch model to the rate equations*, in "Disc. Cont. Dyn. Sys.", vol. 11-1, 2004, p. 1-26.
- [11] B. BIDÉGARAY, F. CASTELLA, E. DUMAS, M. GISCLON. *From Bloch model to the rate equations II: the case of almost degenerate energy levels*, in "Math. Mod. Meth. Appl. Sci.", to appear, 2004.
- [12] E. CANCÈS, F. CASTELLA, P. CHARTIER, E. FAOU, C. L. BRIS, F. LEGOLL, G. TURINICI. *High-order averaging schemes with error bounds for thermodynamical properties calculations by MD simulations*, in "Journal of Chemical Physics", to appear, 2004.
- [13] F. CASTELLA. *The radiation condition at infinity for the high-frequency Helmholtz equation with source term: a wave packet approach*, in "J. Funct. Anal.", to appear, 2004.
- [14] F. CASTELLA, P. CHARTIER, E. FAOU, D. BAYART, F. LEPLINGARD, C. MARTINELLI. *Raman Laser Modeling: Mathematical and Numerical Analysis*, in "Mathematical Modelling and Numerical Analysis", vol.

38-3, 2004, p. 457-475.

- [15] R. CHAN, P. CHARTIER, A. MURUA. *Reversible methods of Runge-Kutta type for Index-2 Differential-Algebraic Equations*, in "Numerische Mathematik", vol. 97, 2004, p. 427-440.
- [16] M. DAUGE, E. FAOU, Z. YOSIBASH. *Plates and shells: Asymptotic expansions and hierarchical models*, in "Encyclopedia for Computational Mechanics", vol. 1, 2004.
- [17] E. FAOU. *Multiscale Expansions for Linear Clamped Elliptic Shells*, in "Communications in PDE", to appear, 2004.
- [18] E. FAOU, E. HAIRER, T.-L. PHAM. *Energy conservation with non-symplectic methods: Examples and counter-examples*, in "BIT", to appear, 2004.
- [19] F. LEPLINGARD, C. MARTINELLI, S. BORNE, L. LORCY, T. LOPEZ, D. BAYART, F. CASTELLA, P. CHARTIER, E. FAOU. *Modeling of multi-wavelength Raman fiber lasers using a new and fast algorithm*, in "IEEE Photonics Technology Letters", to appear, 2004.

Internal Reports

- [20] D. BENEDETTO, F. CASTELLA, R. ESPOSITO, M. PULVIRENTI. *On The Weak-Coupling Limit for Bosons and Fermions*, Submitted to Mathematical Modelling and Numerical Analysis., Technical report, 2004, <http://perso.univ-rennes1.fr/francois.castella/rech.html#recent>.
- [21] E. CANCÈS, F. CASTELLA, P. CHARTIER, E. FAOU, C. L. BRIS, F. LEGOLL, G. TURINICI. *Long-time averaging for integrable Hamiltonian dynamics*, Submitted to Numerische Mathematik., Technical report, 2004, <http://www.irisa.fr/ipso/perso/chartier/#publications>.
- [22] P. CHARTIER, E. FAOU, A. MURUA. *An algebraic analysis of formal methods preserving structures*, Submitted to SIAM J. Numer. Anal., Technical report, 2004, <http://www.irisa.fr/ipso/perso/chartier/#publications>.
- [23] E. FAOU, C. LUBICH. *A Poisson integrator for Gaussian wavepacket dynamics*, Submitted to Computing and Visualization in Science., Technical report, 2004, <http://na.uni-tuebingen.de/na/preprints.shtml>.

Bibliography in notes

- [24] R. D. COALSON, M. KARPLUS. *Multidimensional variational Gaussian wavepackets dynamics with application to photodissociation spectroscopy*, in "J. Chem. Phys.", vol. 93, 1990, p. 3919–3930.
- [25] E. HAIRER. *Geometric integration of ordinary differential equations on manifolds*, in "BIT", vol. 41, 2001, p. 996–1007.
- [26] E. HAIRER, C. LUBICH, G. WANNER. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer Series in Computational Mathematics 31, Springer, Berlin, 2002.
- [27] E. HAIRER, G. WANNER. *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems*, Springer Series in Computational Mathematics 14, 2, Springer-Verlag, Berlin, 1996.

- [28] E. HELLER. *Time dependent approach to semiclassical dynamics*, in "J. Chem. Phys.", vol. 62, 1975, p. 1544–1555.
- [29] A. ISERLES, H. Z. MUNTHE-KAAS, S. P. NØRSETT, A. ZANNA. *Lie-group methods*, in "Acta Numerica", 2000, p. 215–365.
- [30] C. LUBICH. *On variational approximations in quantum molecular dynamics*, in "Math. Comp.", to appear.
- [31] C. LUBICH. *A variational splitting integrator for quantum molecular dynamics*, in "Appl. Numer. Math.", vol. 48, 2004, p. 355–368.
- [32] F. A. POTRA, W. C. RHEINBOLDT. *On the numerical solution of Euler-Lagrange equations*, in "Mech. Struct. & Mech.", vol. 19, 1991, p. 1–18.
- [33] J. M. SANZ-SERNA, M. P. CALVO. *Numerical Hamiltonian Problems*, Chapman & Hall, London, 1994.